

MATERIALS PROPERTIES NUMERICAL DATABASE SYSTEM

ESTABLISHED AND OPERATIONAL AT CINDAS/PURDUE UNIVERSITY

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Abstract

A computerized comprehensive numerical database system on the mechanical, thermophysical, electronic, electrical, magnetic, optical, and other properties of various types of technologically important materials such as metals, alloys, composites, dielectrics, polymers, and ceramics has been established and operational at the Center for Information and Numerical Data Analysis and Synthesis (CINDAS) of Purdue University. This is an on-line, interactive, menu-driven, user-friendly database system. Users can easily search, retrieve, and manipulate the data from the database system without learning special query language, special commands, standardized names of materials, properties, variables, etc. It enables both the direct mode of search/retrieval of data for specified materials, properties, independent variables, etc. and the inverted mode of search/retrieval of candidate materials that meet a set of specified requirements (which is the computer-aided materials selection). It enables also tabular and graphical displays and on-line data manipulations such as units conversion, variables transformation, statistical analysis, etc. of the retrieved data. The development, content, accessibility, etc. of the database system are presented and discussed.

Introduction

The Center for Information and Numerical Data Analysis and Synthesis (CINDAS) was founded at Purdue University on 1 January 1957, originally as the Thermophysical Properties Research Center (TPRC). It is dedicated to the advancement of science, engineering, and technology through better knowledge of the properties of materials.

For 30 years since its inception CINDAS has been extracting and compiling material property data from worldwide scientific and technical literature and has been evaluating, analyzing, correlating, and synthesizing the compiled experimental data to generate reliable reference data (the so-called recommended values). As a result, CINDAS has developed a number of comprehensive and authoritative numerical databases. The existing databases established at CINDAS contain a total of over 125,000 sets of data* on the properties of all types of technologically important materials, which will be detailed later.

Since 1972 CINDAS has been developing a computerized "Materials Properties Numerical Database System." The data already available at CINDAS are gradually and selectively being computerized. The new data for databases developed in recent years are, however, all fully computerized.

One of the salient features of the databases developed by CINDAS is that each database contains both the experimental data compiled from the worldwide literature and the evaluated reliable reference data (recommended values) for selected more important materials (as resources permit) resulting from critical evaluation, analysis, correlation, and synthesis of the compiled data, as CINDAS has always considered the quality and credibility of the data in a database to be of utmost importance.

The major databases in the materials properties numerical database system at CINDAS as well as their development, accessibility, etc. are presented and discussed in the following sections.

Development, Accessibility, and Characteristics of the Database System

The computerized numerical database system on materials properties established at CINDAS is an on-line, interactive, menu-driven, user-friendly system. A user can easily search, retrieve, and manipulate the data from the database system without learning special query language, special commands, standardized names of materials, properties, variables, etc. This on-line database system is managed by a data base management system (DBMS) developed by CINDAS over the years particularly for the management and operation of numerical databases. This unique DBMS is well known for its user-friendliness and instant responsiveness and in the ease and versatility of operation in dealing with numerical databases.

*One set of data consists of numerical data points (as a function of temperature and/or other independent variable) and pertinent information on the specification and characterization of the test materials and on the method and conditions of the property measurement, plus the data source reference.

This database system enables the on-line interactive search/retrieval of at least the following:

- (1) Numerical property data in tabular and graphical forms and pertinent information on the test material and property measurement for specified materials, properties, independent variables, etc. (direct mode).
- (2) Candidate materials that meet a set of specified requirements (inverted mode), which is the so-called computer-aided materials selection (CAMS).
- (3) General descriptions of individual materials including composition, crystalline structures, synonyms, trade names, manufacturing processes, unusual properties and behavior, recommended applications, etc. (these general descriptions of materials are in addition to the specific descriptions and characterizations of individual test materials which are recorded together with the numerical data as part of the individual data sets).
- (4) Definitions of material properties and other relevant technical terms.
- (5) Summaries of ASTM test methods for material property measurements and their significance.
- (6) Bibliographic citations of references to specified materials/properties combinations or authors.

It enables also the on-line data manipulations such as units conversion, variables transformation, statistical analysis, etc. of the retrieved data.

The database system contains a number of databases and each database is on a large group of materials. The development of each database involves:

- (1) The in-depth cognizance and acquisition of the relevant worldwide scientific and technical literature.
- (2) The exhaustive extraction and compilation of data and information from the acquired pertinent research documents.
- (3) The critical evaluation, analysis, correlation, and synthesis of the compiled experimental data to generate reliable reference data.
- (4) The computerization of both the experimental data and the CINDAS-generated reliable reference data to create various data files.
- (5) The development of various ancillary files necessary for the database.
- (6) The integration of the various data files to establish an operational computerized database.

As the material property data recorded in the scientific and technical literature are often conflicting, widely diverging, and subject to large uncertainty, the literature data are critically evaluated and analyzed to generate reliable reference data. The availability of both the critically evaluated reference data and the experimental data in the database is one of the salient features of CINDAS' comprehensive materials properties database system. The methodology of critical evaluation, analysis, correlation, and synthesis of material property data used at CINDAS has been discussed in detail elsewhere [1]. Basically, it involves critical evaluation of the validity of the available data and related information, judgment on the reliability and accuracy of the data, resolution and reconciliation of disagreements in conflicting data (distinguishing first the real difference in data due to sample difference from the disagreement in data due to

experimental error), correlation of data in terms of various affecting parameters (sometimes in reduced forms using the principle of corresponding states), curve fitting with theoretical or empirical equations, synthesis of the often fragmentary data (sometimes by combining the available data with the values derived from the data on related properties or related materials) to generate a fuller range of coverage of internally consistent values, comparison of the resulting values with theoretical predictions or with results calculated from theoretical relationships, etc.

As an example to illustrate our work on the critical evaluation and analysis of experimental data, Figure 1 shows part of the available experimental data as well as CINDAS' recommended values for the thermal conductivity of tungsten. It can be observed from Figure 1 that a large portion of the experimental data are conflicting, widely diverging, and subject to large uncertainty, and the spread of data is over three hundred percent. The true values of the thermal conductivity of tungsten had not been known even with the availability of over 400 publications on this subject published beginning in 1914 until CINDAS critically evaluated and analyzed the discordant experimental data and generated the recommended reference values in 1964 as shown in the figure. These CINDAS' recommended values have been recognized as national standard reference data. Similarly, Figure 2 shows the available experimental data and CINDAS' recommended values for the thermal diffusivity of tungsten and that the lower portion of the experimental data are utterly erroneous, being about five times too low.

Our work on the correlation and synthesis of experimental data is illustrated by Figures 3 to 8. Figure 3 shows the available experimental data on the thermal conductivity of aluminum + copper alloys, which are very limited, fragmentary, and conflicting. Based on the results of evaluation and analysis of these thermal conductivity data and on CINDAS' recommended values for the electrical resistivity and the thermoelectric power of these alloys, the full-range recommended values for the thermal conductivity of these alloys were generated as shown in Figure 4.

Figure 5 presents the recommended values for the electrical resistivity of iron + nickel alloys as the final results of correlation and synthesis of the available experimental data which are not shown. Similarly, Figure 6 presents the recommended values for nickel + iron alloys. The pronounced effect of the ferromagnetic-paramagnetic transition on the electrical resistivity of the alloys at the Curie temperature is strikingly shown in the two figures. These two sets of recommended values together cover the thermal conductivity of the entire iron-nickel alloy system for all alloy compositions and all temperatures.

Figure 7 shows the recommended values for the absolute thermoelectric power of copper-nickel alloy system covering all alloy compositions and all temperatures up to 1,300 K. The effect of the ferromagnetic-paramagnetic transition on the thermoelectric power of the alloys is also clearly shown.

As an example to show the results of our work on mechanical properties, Figure 8 shows a stress-fracture map for 316 stainless steel such that we have extended the tensile stress versus failure time curves into the short-time domain, in which data from constant-load rapid-heating testing as well as from constant strain-rate testing after rapid heating are shown also. Such a stress-fracture map presents a considerable body of mechanical property information in a single figure wherein the regions for all the material fracture mechanisms under load are indicated, including ductile transgranular fracture, transgranular creep fracture, intergranular creep fracture, rupture, and mixed mode of fracture.

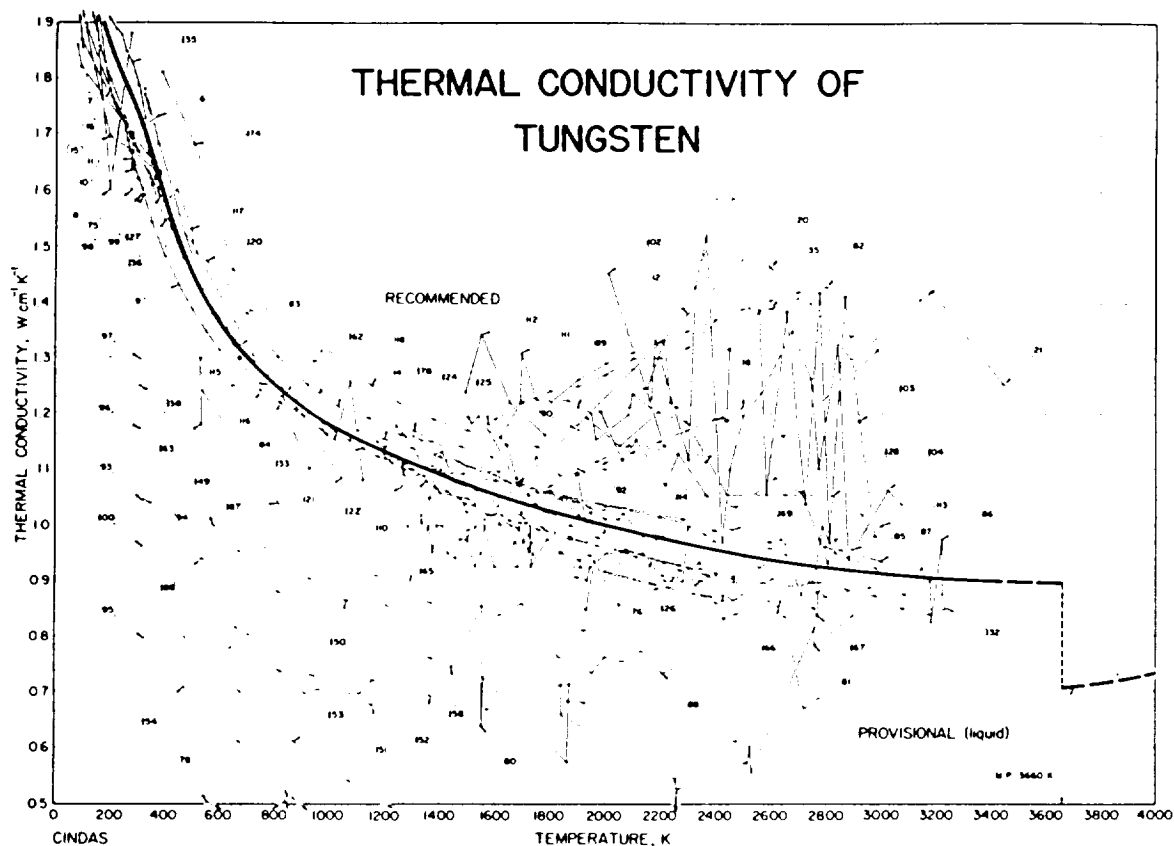


Figure 1. Experimental data and recommended values for the thermal conductivity of tungsten.

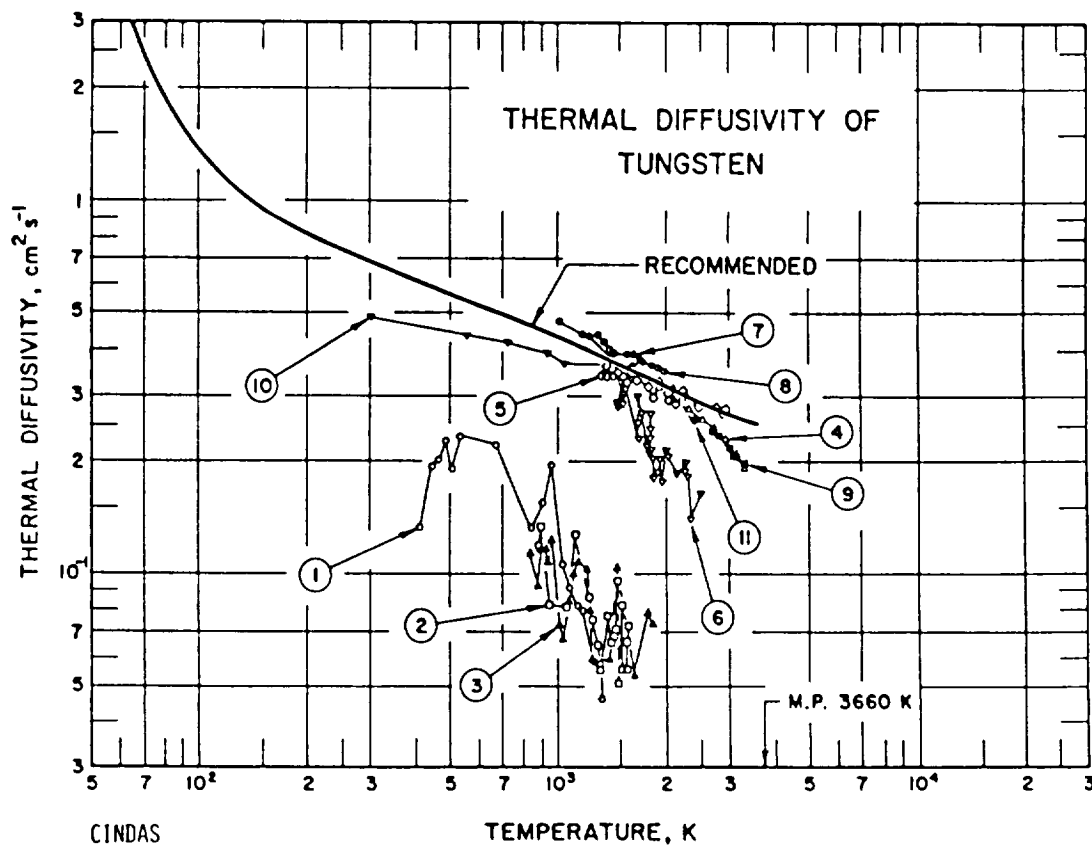


Figure 2. Experimental data and recommended values for the thermal diffusivity of tungsten.

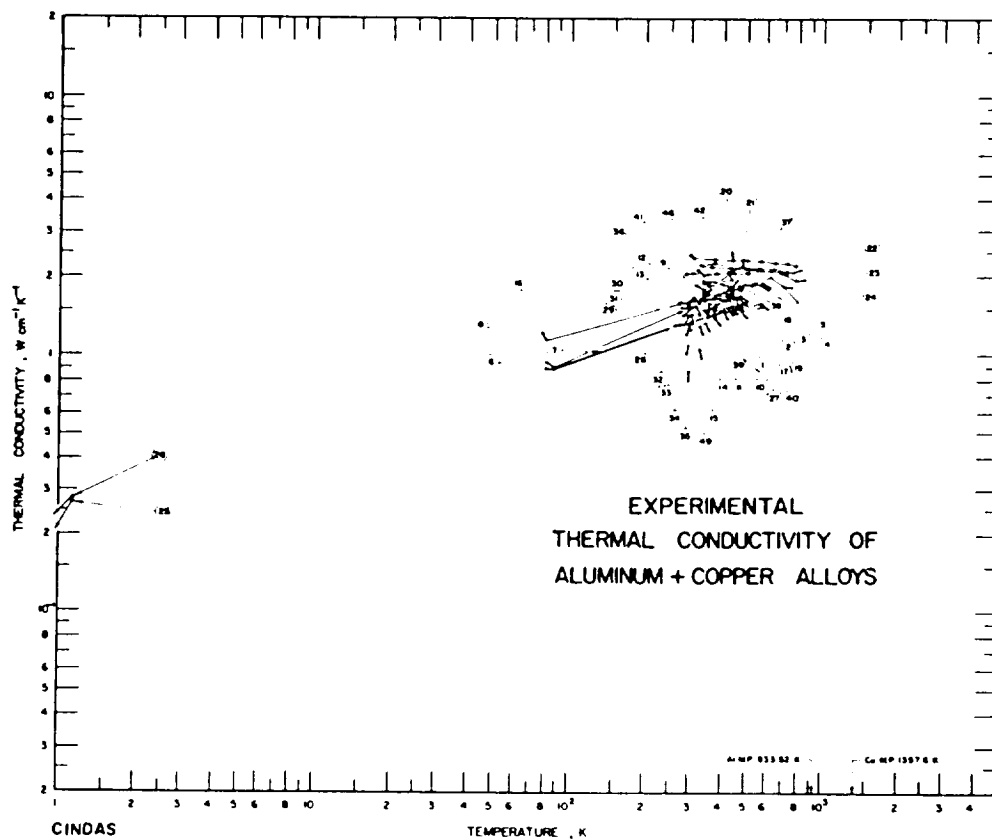


Figure 3. Experimental data on the thermal conductivity of aluminum + copper alloys.

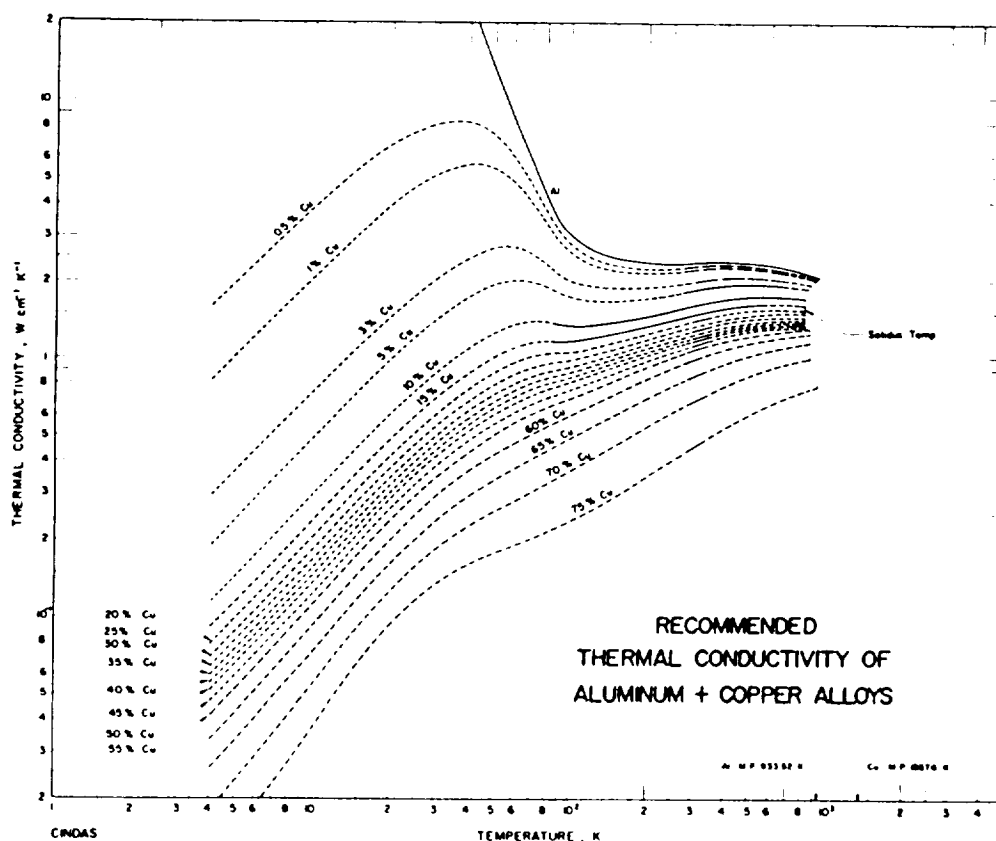


Figure 4. Recommended values for the thermal conductivity of aluminum + copper alloys.

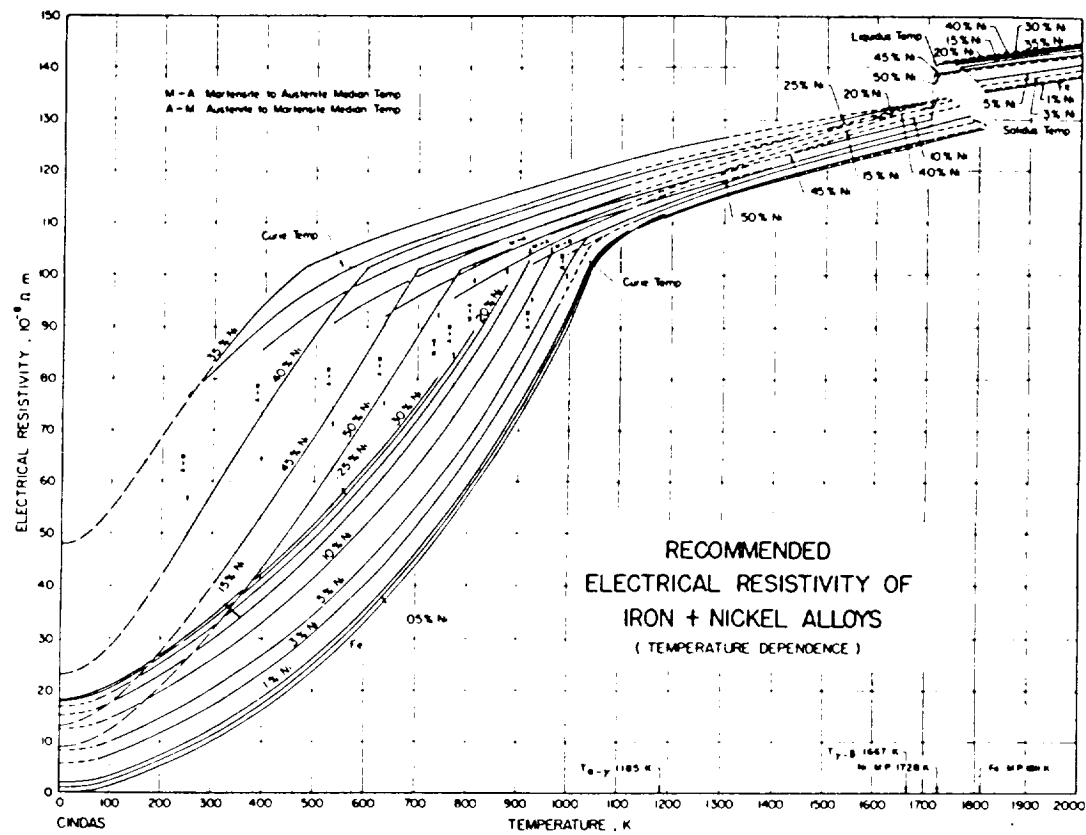


Figure 5. Recommended values for the electrical resistivity of iron + nickel alloys.

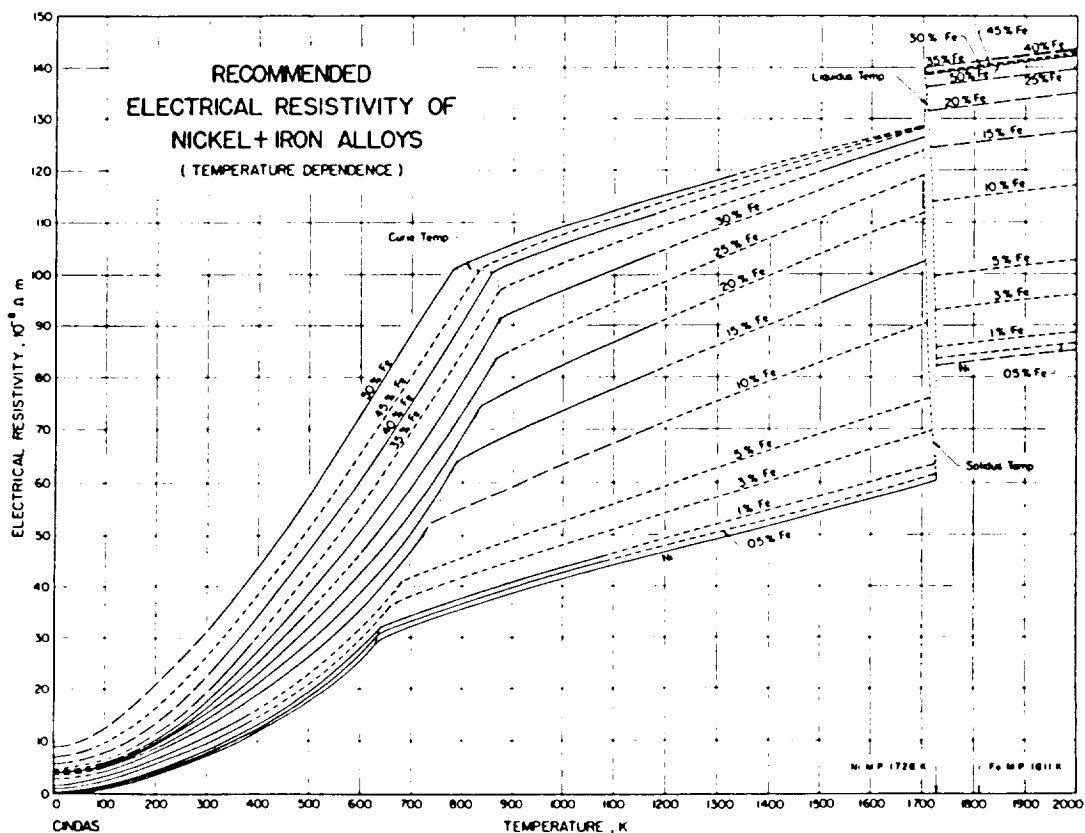


Figure 6. Recommended values for the electrical resistivity of nickel + iron alloys.

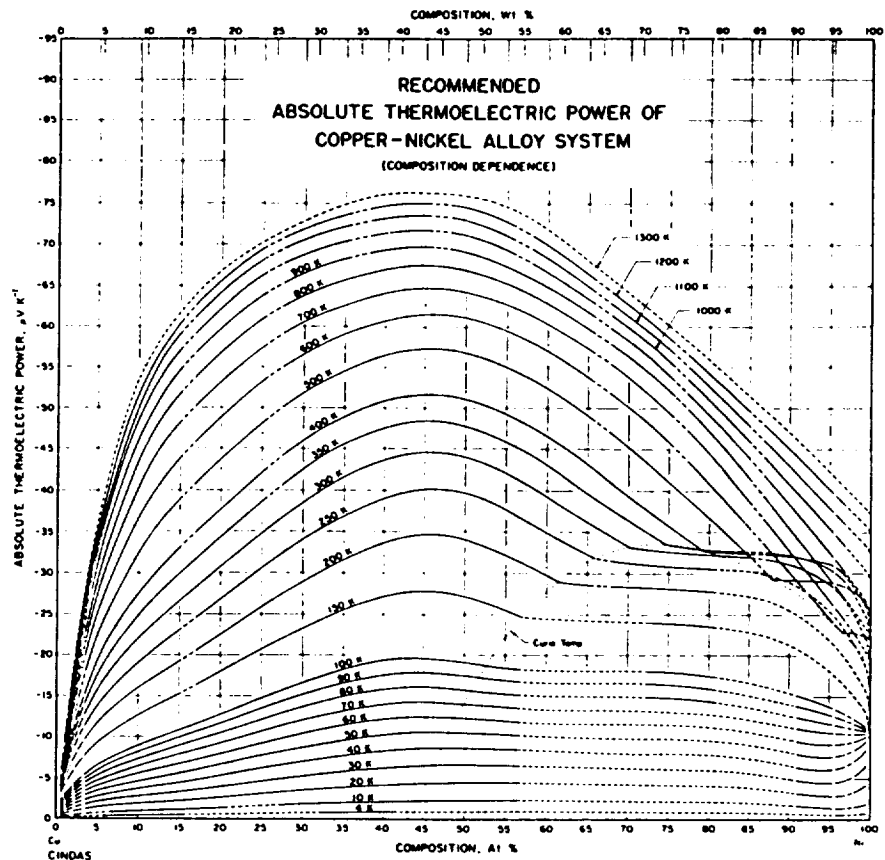


Figure 7. Recommended values for the absolute thermoelectric power of copper-nickel alloy system.

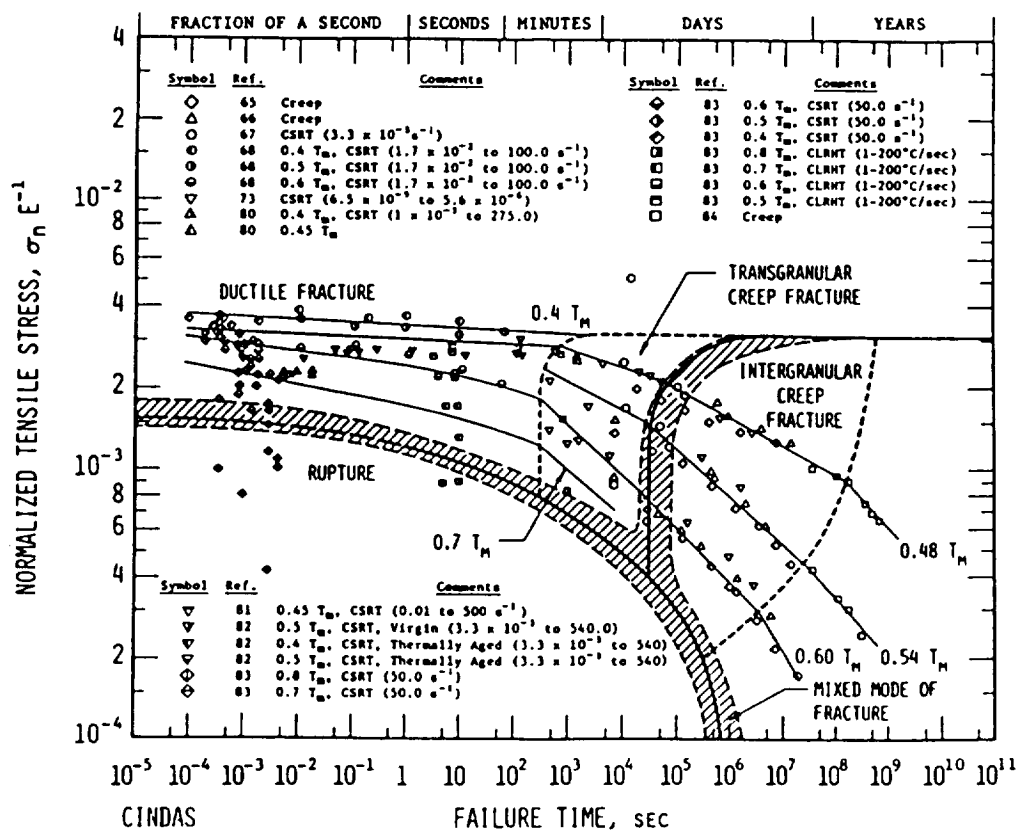


Figure 8. Stress-fracture map for 316 stainless steel extended to short-time domain.

As mentioned before, our critically evaluated reference data (recommended values) as well as the experimental data compiled from worldwide literature are all stored in the various databases.

Contents of the Materials Properties Numerical Database System

This database system contains a number of numerical databases. Major databases that have been developed at CINDAS are briefly discussed below.

1. High Temperature Materials Properties Database

This database is developed by the DoD High Temperature Materials - Mechanical, Electronic and Thermophysical Properties Information Analysis Center (HTMIAC), which is operated by CINDAS for the U.S. Department of Defense (DoD) under the sponsorship of the Office of the Undersecretary of Defense Research and Engineering. So far this database contains about 12,000 sets of data on the thermophysical, thermoradiative, optical, electronic, and mechanical properties of aerospace structural composites and metals and infrared detector/sensor materials (about 82% of the data are extracted from worldwide open literature and unclassified, unlimited-distribution U.S. Government reports). All the data in this database have been computerized.

These 12,000 sets of data cover 280 varieties of aerospace structural composites (including 32 varieties of carbon/carbon composites, 63 varieties of carbon/phenolic composites, 16 varieties of fiberglass/epoxy composites, 9 varieties of graphite/bismaleimide composites, 118 varieties of graphite/epoxy composites, 23 varieties of graphite/polyimide composites, 7 varieties of Kevlar/epoxy composites, and 12 varieties of silica/phenolic composites), 102 varieties of composite constituents, 120 varieties of aerospace structural alloys, and 53 varieties of infrared detector/sensor materials [2]. Additional aerospace structural materials and infrared detector/sensor materials will be covered in the future.

Since material property data are meaningful only if adequate information on the test material and on the property measurement is also provided, each set of data in our database consists of numerical data points (as a function of temperature and/or other independent variable) and pertinent information on the specification and characterization of the test material and on the method and conditions of the property measurement, such as composition, purity, density, porosity, microstructure, material construction configuration, material processing, sample preparation, specimen geometry and dimensions, material history, heat treatment, cold working, surface condition, producer, supplier, method of measurement, test environment, heat flow direction, heating rate, heat-up time, heat-up temperature, holding time at temperature, type of heat source, and loading rate, insofar as these are contained in the original document.

As an example to show the data and information stored in this computerized database, one set of data on the thermal linear expansion along a specific direction of a particular sample of Hercules AS/3501-6 graphite/epoxy composite is shown in Table I.

The compiled experimental data for selected priority materials and properties have been and are being critically evaluated and analyzed to generate recommended values, which are also included in the database. Furthermore, in order to support the DoD high energy laser community for their studies of the effects of lasers on materials, structures, and detectors as well as for the vulnerability, survivability, and hardening assessments, we have been generating high temperature, high heating rate,

Table I. Example of One Set of Data on the Thermal Linear Expansion of
a Particular Sample of Hercules AS/3501-6 Graphite/Epoxy
Composite along a Specific Direction in the High Temperature
Materials Properties Database

MATERIAL: HERCULES AS/HERCULES 3501-6 HTMIAC/CINDAS
PROPERTY: THERMAL LINEAR EXPANSION DATA SET 1

COMPOSITION :
65.0 WEIGHT PERCENT HERCULES MAGNAMITE AS GRAPHITE FIBER
35.0 WEIGHT PERCENT HERCULES 3501-6 EPOXY

SUPPLIER/PRODUCER/FABRICATOR :
PREPREG TAPES FROM HERCULES, INC.

COMPOSITE MATERIAL ARCHITECTURE, FIBER DESCRIPTION :
REINFORCEMENT ARCHITECTURE : 2D (0)
NUMBER OF PLIES : 5

PROCESSING HISTORY, MATRIX DESCRIPTION :
CURING/DENSIFICATION SEQUENCE :
PREPREG TAPE CUT TO SIZE AND 5 PLIES LAID UP BY HAND TO PROPER
DIMENSIONS OF 12 INCH X 24 INCH X 0.025 INCH ON RELEASE-AGENT
COATED STAINLESS STEEL PLATE; ON THE TOP WERE PLACED IN ORDER,
A LAYER OF RELEASE CLOTH, A LAYER OF OPEN CELL FOAM/RANDOM FIBER
BLEEDER CLOTH, AND A LAYER OF POLYETHYLENE FILM; ENTIRE UNIT WAS
PLACED IN BLANKET PRESS AND CURED.
CURED AT 100 C FOR ONE HOUR, AND AT 177 C FOR THREE HOURS.

ADDITIONAL PREPARATION/CONDITIONING :
ADDITIONAL CONDITIONING/PREPARATION : MOISTURE
DESCRIPTORS-TEXTUAL :
MOISTURE CONDITIONED AT 98 PERCENT RELATIVE HUMIDITY FOR 30 DAYS
AT 65.5 C (1.69 PERCENT AVERAGE MOISTURE CONTENT).

SPECIMEN IDENTIFICATION :
DIMENSIONS (GEOMETRY) :
LENGTH 57.2 MM
WIDTH 6.35 MM
ORIENTATION WITH RESPECT TO MATERIAL : INTERLAMINAR, THROUGH THICKNESS

MEASUREMENT/EVALUATION METHOD :
NAME/DESCRIPTION :
QUARTZ DILATOMETER EMPLOYING DAYTRONIC MODEL DS200 LVDT.
MEASUREMENT ACCURACY WAS 0.0001 INCH WITH 0.1 PERCENT ERROR.
THE QUARTZ PUSH-ROD EXERTED A FORCE OF 9 GRAMS.

MEASURED/EVALUATED PROPERTIES :
X : TEMPERATURE K
Y : THERMAL LINEAR EXPANSION PERCENT

Table I (Continued)

DATA POINTS :

X	Y	REMARKS:
2.081E+02	-1.810E-01	SPECIMEN G4
2.306E+02	-1.350E-01	
2.673E+02	-6.990E-02	
2.868E+02	-3.110E-02	
3.135E+02	3.040E-02	
3.378E+02	7.380E-02	
3.638E+02	1.420E-01	
2.086E+02	-1.900E-01	SPECIMEN G5
2.306E+02	-1.420E-01	
2.673E+02	-8.960E-02	
2.861E+02	-3.490E-02	
3.140E+02	3.650E-02	
3.376E+02	1.000E-01	
3.644E+02	1.590E-01	
2.081E+02	-1.740E-01	SPECIMEN G6
2.299E+02	-1.320E-01	
2.673E+02	-8.050E-02	
2.868E+02	-2.960E-02	
2.980E+02	-7.000E-04	
3.140E+02	4.260E-02	
3.378E+02	8.900E-02	
3.644E+02	1.510E-01	
2.031E+02	-1.880E-01	SMOOTH VALUES (1.87 PERCENT MOISTURE)
2.231E+02	-1.580E-01	
2.431E+02	-1.250E-01	
2.631E+02	-8.700E-02	
2.731E+02	-6.700E-02	
2.831E+02	-4.700E-02	
3.031E+02	-2.000E-03	
3.231E+02	4.600E-02	
3.431E+02	9.800E-02	
3.631E+02	1.540E-01	

DATA -- COMMENTS :

AVERAGE MOISTURE CONTENT WAS 1.69 PERCENT FOR THE MEASURED DATA,
AND WAS 1.87 PERCENT FOR VALUES OBTAINED FROM A POLYNOMIAL FIT.
THERMAL LINEAR EXPANSION (TLE) = $-6.745E-02 + 2.047E-03T + 4.546E-08T^2$ FOR TLE IN PERCENT AND T IN CELSIUS.

REFERENCE:

MOISTURE AND THERMAL EXPANSION OF COMPOSITE MATERIALS.
CAIRNS, D. S. AND ADAMS, D. F.
UNIV. WYOMING, MECH. ENG. DEPT. REPT. UWME-DR-101-104-1
204 PP., 1981.
(AD-A109 131, ARO-16370.5-MS)

and/or high strain rate data through analysis, correlation, synthesis, and extrapolation of the available experimental data for moderate temperatures, low heating rates, and/or low strain rates, and through theoretical estimation based on our knowledge gained by intensive studies of the effects of high heating rates and high strain rates on material properties. All these efforts add much value to the existing data and greatly enhance this database.

The properties covered by this database are listed below:

(A) Thermophysical, thermoradiative, optical, and electronic properties:

- (1) Ablation energy
- (2) Ablation temperature
- (3) Absorptance
- (4) Absorption coefficient
- (5) Boiling point
- (6) Density
- (7) Electrical resistivity
- (8) Emittance
- (9) Heat capacity
- (10) Heat of fusion
- (11) Heat of vaporization
- (12) Melting point
- (13) Reflectance
- (14) Refractive index
- (15) Thermal conductivity
- (16) Thermal diffusivity
- (17) Thermal linear expansion
- (18) Transmittance

(B) Mechanical properties:

- (1) Compressive modulus
- (2) Compressive strain at fracture
- (3) Compressive strength, ultimate
- (4) Compressive strength, yield
- (5) Elastic constants
- (6) Elongation
- (7) Energy release rate
- (8) Flexural modulus
- (9) Flexural strength
- (10) Fracture toughness
- (11) Hardness
- (12) Impact energy
- (13) Poisson's ratio
- (14) Reduction in area
- (15) Shear modulus
- (16) Shear modulus, in-plane
- (17) Shear strain at fracture
- (18) Shear strength, in-plane
- (19) Shear strength, interlaminar
- (20) Shear strength, ultimate
- (21) Shear strength, yield
- (22) Stress-strain curves, compression
- (23) Stress-strain curves, shear
- (24) Stress-strain curves, tension
- (25) Tensile modulus
- (26) Tensile strain at fracture

- (27) Tensile strength, ultimate
- (28) Tensile strength, yield

This database is continually being updated and expanded by HTMIAC/CINDAS.

2. Engineering Materials Properties Database

This database has been developed by CINDAS since 1957 through multiple supports of DoD, other Government Agencies, numerous industrial organizations, research institutes and foundations, professional societies, and Purdue University. It contains approximately 100,000 sets of data on the following properties of more than 7,000 materials*:

(A) Thermophysical and thermoradiative properties:

- (1) Accommodation coefficient
- (2) Prandtl number
- (3) Solar absorptance to hemispherical total emittance ratio
- (4) Specific heat
- (5) Thermal absorptance
- (6) Thermal conductivity
- (7) Thermal diffusivity
- (8) Thermal emittance
- (9) Thermal linear expansion
- (10) Thermal reflectance
- (11) Thermal transmittance
- (12) Thermal volumetric expansion
- (13) Viscosity

(B) Electronic, electrical, magnetic, and optical properties:

- (1) Absorption coefficient
- (2) Dielectric constant
- (3) Dielectric strength
- (4) Electrical resistivity
- (5) Hall coefficient
- (6) Magnetic susceptibility
- (7) Refractive index
- (8) Thermoelectric properties
- (9) Work function

The mechanical properties of selected alloys are also covered.

The over 7,000 selected materials covered in this database are from the following groups of materials:

- (1) Metallic elements
- (2) Graphites and nonmetallic elements
- (3) Ferrous alloys (15 groups)
- (4) Nonferrous alloys (41 groups)
- (5) Intermetallic compounds
- (6) Inorganic compounds
- (7) Organic compounds
- (8) Ceramics
- (9) Cermets

*It should be understood that the number of properties covered by the available data for each of the materials varies greatly, ranging from almost all to only few of the properties listed.

- (10) Glasses
- (11) Polymers
- (12) Composites
- (13) Applied coatings
- (14) Systems
- (15) Insulations
- (16) Fabrics
- (17) Natural substances
- (18) Biological materials

However, only a small portion of the data in this database have been computerized and the remaining major portion of the data are yet to be computerized.

In addition to experimental data extracted and compiled from worldwide scientific and technical literature, this database contains also many thousands of evaluated data sets (sets of recommended values).

3. EPRI Database on Dielectric Materials

This database is developed by CINDAS under the sponsorship of the Electric Power Research Institute (EPRI) [3]. It is to serve as a centralized source of technical, commercial, and applications data on dielectric materials, and to disseminate such data directly to the fingertips of engineers, scientists, designers, researchers, etc. through computer terminals across the nation.

The database contains data and information on the following properties (or information items) of electrical insulating liquids, solids, gases, and combinations thereof:

- (1) Electrical properties
- (2) Physical properties
- (3) Chemical properties
- (4) Thermal properties
- (5) Optical and thermoradiative properties
- (6) Mechanical properties
- (7) Flammability properties
- (8) Aging and degradation information
- (9) Health hazard and environmental effects
- (10) Processability and manufacturing information
- (11) Recommended applications
- (12) Producer, supplier, and availability information
- (13) Price range and other commercial information

This database is fully computerized and on-line operational. It covers so far 371 dielectric liquids, 1,120 dielectric solids, 12 dielectric gases, 271 properties, and 76 independent variables.

Although the establishment of this database is for the benefit of the electric power industry, its manufacturers and suppliers, and the dielectric research and development community, data on dielectric materials are very much needed in many other areas of applications, such as in the field of nuclear fusion and in high voltage dc and pulsed power applications in advanced weapons systems and electronic military hardware (such as high power laser weapons).

4. Thermophysical Properties Database on Fluids

This database is fully computerized and contains data and information on 13 properties of some 300 fluids.

Thermophysical properties of fluids are important for all applications involving heat, mass, and/or momentum transfer using fluid as a medium, including also military applications such as the design of engine cooling systems, lubricating systems, fuel systems, and combustion and exhaust systems of military vehicles, tanks, airplanes, warships, etc.

5. Thermophysical and Mechanical Properties Database on Rocks and Minerals

This database contains data and information on the mechanical, thermophysical, electrical, magnetic, and optical properties of 155 types of rocks and 293 minerals.

The data and information on the properties of rocks and minerals are important for various applications such as in the site selection, design, and construction of underground nuclear waste disposal facilities, hardened missile silos, nuclear test sites, underground power plants, and deep underground defense facilities. In the geosciences, such data are important for the calculation of accurate values for heat flow in the earth's crust, which are needed to obtain a better understanding of the earth's history and its current makeup. Rock property data are also needed for the evaluation of the theories on sea floor spreading and plate tectonics in addition to supplying details for the substantial deep sea rock coring program. Geothermal power generation techniques and earthquake prediction analysis both depend to some degree on thermophysical properties and heat flow of rock masses.

6. SRC Packaging Materials Database

This database is being developed by CINDAS under the sponsorship of the Semiconductor Research Corporation (SRC). It covers the thermal, electrical, physical, mechanical, and other properties of selected semiconductors, metals, alloys, nonmetallic elements, ceramics, inorganic compounds, epoxies, plastics, composites, and fluids.

This database is intended to serve the microelectronic packaging needs of the semiconductor/electronics industry for comprehensive, reliable data on packaging materials.

References

1. C. Y. Ho and Y. S. Touloukian, "Critical Evaluation, Correlation, Analysis, and Synthesis of Thermophysical, Electrical, Thermoelectric, and Optical Properties Data," in Proceedings of the Eighth Symposium on Thermophysical Properties (J. V. Sengers, ed.), Vol. 2 (New York, NY: American Society of Mechanical Engineers, 1982), 419-430.
2. C. Y. Ho and R. H. Bogaard, "Materials, Properties, Parameters, and Independent Variables Covered in HTMIAC's Computerized High Temperature Materials Properties Data Base," (HTMIAC Report 4, DOD High Temperature Materials Information Analysis Center, Purdue University, 1986).
3. C. Y. Ho, H. H. Li, and Nirmal Singh, "Establishment of a Computerized Comprehensive On-Line Intelligent Data Base on Dielectric Materials," in Proceedings of the 17th Electrical/Electronics Insulation Conference (New York, NY: The Institute of Electrical and Electronics Engineers, Inc., 1985), 230-236.